bio-protocol Preprint

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Generate dot surface of the channel hole for CALHM1 using HOLE program

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An abbreviated version of this protocol was published in Science Advances in Jul 2020

Cryo-EM structure of the calcium homeostasis modulator 1 channel

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Detailed protocol

1. Install the HOLE program following the instruction from the HOLE web site (http://www.holeprogram.org/doc/index.html).
2. Prepare the input file. The screenshot of the input file containing the setting parameters for hole calculation of CALHM1 is attached as an uploaded file.
3. Running HOLE by typing command “hole < hole.inp > hole.out “ in the shell.
4. Run command “sph_process -dotden 50 hole_out.sph dotsurface.qpt” to produce a dot surface for hole_out.sph file, which was generated by step 3.
5. Run command “qpt_conv dotsurface.qpt” to convert the qpt file that generated by step 4, and choose the output format. In our lab, we usually use the Rasmol format (Option R) and see the dot surface in PyMol.
6. Extract the radius information using command “egrep "mid-|sampled" hole.out > hole_out.tsv", and plotting the 2D graph of pore radius by MS-Excel or other spreadsheet software.

Related files

hole_input.png

How to cite:（Readers should cite both the Bio-protocol preprint and the original research article where this protocol was used）

1. Yang, X. and Shen, Y. (2021). Generate dot surface of the channel hole for CALHM1 using HOLE program. Bio-protocol Preprint. bio-protocol.org/prep938.
2. Ren, Y., Wen, T., Xi, Z., Li, S., Lu, J., Zhang, X., Yang, X. and Shen, Y.(2020). Cryo-EM structure of the calcium homeostasis modulator 1 channel . Science Advances 6(29). DOI: 10.1126/sciadv.aba8161

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